

Amendments to the Claims:

This listing of claims will replace all prior versions, and listings, of claims in this application.

Listing of Claims:

- 1-4. (Canceled).
5. (Withdrawn) A mixture comprising a crystalline biological target molecule and a plurality of core fragments selected from a library of core fragments, wherein at least 40% of the plurality of core fragments comprise an anomalous dispersion substituent.
- 6-49. (Canceled).
50. (Currently Amended) A method of designing a lead candidate having biophysical or biochemical activity against a biological target molecule, comprising the steps of:
- a) Combining a crystalline biological target molecule with a mixture comprising at least two compounds, wherein at least one of said compounds comprises a substituent having anomalous dispersion properties comprising bromine;
 - b) Determining the structure of at least one of said compounds in association with said biological target molecule using x-ray crystallographic analysis; and
 - c) Selecting information from the structure to design said lead candidate.
- 51-56. (Canceled).
57. (Currently Amended) The method of claim 50, wherein said ~~identifying-determining~~ of said at least one compound of step b uses the anomalous dispersion properties of said substituent.
58. (Withdrawn) The mixture of claim 4, wherein about half of said core fragments in said mixture comprise an anomalous dispersion substituent.

- 59. (Withdrawn) The mixture of claim 4, wherein said plurality of core fragments comprises at least 10 core fragments.
- 60. (Withdrawn) The mixture of claim 4, wherein said anomalous dispersion substituent is bromine.
- 61. (Previously Presented) The method of claim 50, wherein said selecting information comprises selecting computed deformation energy of binding information, volume overlap information, induced fit information, computed electrostatic interaction information, and/or computed binding free energy information.
- 62. (Previously Presented) The method of claim 50, wherein said selecting information comprises selecting computed energy minimization energy and/or computed molecular dynamics information.
- 63. (Cancelled)
- 64. (Withdrawn) A method of identifying a core fragment comprising an anomalous dispersion substituent, said core fragment bound to a crystalline biological target molecule, wherein said identifying of said core fragment uses the anomalous dispersion properties of said anomalous dispersion substituent.
- 65. (Withdrawn) The method of claim 64, wherein said core fragment forms part of a library of core fragment compounds.
- 66. (Withdrawn) The method of claim 64, wherein said anomalous dispersion substituent is bromine.
- 67. (Withdrawn) A method of screening a plurality of core fragments for a core fragment that binds to a biological target molecule, wherein at least one of said compounds comprises a substituent having anomalous dispersion properties, said method comprises the steps of:

a. soaking a crystal comprising the biological target molecule in a solution comprising said plurality of core fragments; and

b. identifying a compound bound to said biological target molecule using x-ray crystallographic analysis.

68. (Withdrawn) The method of claim 67, wherein said substituent is bromine.

69. (Withdrawn) The method of claim 67, wherein said identifying of said compound of step b uses the anomalous dispersion properties of said substituent.